ARTIFICIAL INTELLIGENCE IN THEORETICAL MATERIALS SCIENCE

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In theoretical materials science, whose main mission is to develop new materials and to predict how the properties of already existing materials change under operation conditions, there are two large trends – multiscale modeling and informatics of materials. The first is slow but accurate, and the second is fast but not so accurate. The first relies on theory that may be imperfect, while the second is based on the artificial intelligence assisted analysis of material properties databases that are, as a rule, incomplete and dissimilar, or absent at all for new materials. In multiscale modeling, there is room for artificial intelligence too. For example, condensed matter calculations by the methods of quantum theory may be accelerated with the use of machine-learning-based interaction models that are quite applicable on a higher scale of atomistic simulation. The future must certainly join these two approaches into a unique one where databases for artificial intelligence are generated or extended with multiscale-modeling assisted digital tools. Here prospects open for development of new materials: electrides for advanced batteries, low-dimensional magnets for spintronics, Kitaev spin-liquid magnets for quantum computers, record radiation-resistant materials for new generations of nuclear reactors, as well as new weapons-grade materials.